Phosphonic acid, bis(1-methylethyl) ester

1809-20-7 | DTXSID7061988

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.90e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.41e-01

Confidence level: 6.49e-01

Nearest Neighbors from the Training Set

Image not found
Diisopropyl methylphosphonate
Measured: 8.88e-01
Predicted: 4.69e-01

Image not found
Dibutyl phosphite
Measured: 3.76e-02
Predicted: 4.20e-02

Image not found
Triethyl phosphate
Measured: 2.74
Predicted: 1.41

Image not found
Dimethyl methylphosphonate
Measured: 8.06
Predicted: 6.36